

# Organometallic Lanthanide Single-Ion Magnets on Surfaces

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Single-ion magnets (SIMs) are molecular complexes containing only a single transition metal or lanthanide ion, which exhibit magnetic hysteresis of purely molecular origin without the need of long-range magnetic order [1,2]. Organometallic lanthanide SIMs are a special class of these materials. In recent years, this field has seen much activity with the most prominent member being the record-breaking, high-blocking-temperature dysprosocenium SIM [3,4].

In this work we study two different sandwich-type erbium-based SIMs built from the anionic ligands cyclooctatetraenide (COT<sup>2-</sup>) and pentamethyl-cyclopentadienide (Cp<sup>-</sup>), namely Cp<sup>\*</sup>ErCOT [5] and [K(18-crown-6)]<sup>+</sup>[Er(COT)<sub>2</sub>]<sup>-</sup> [6]. Our experiments on submonolayers of these SIMs on the Ag(100) surface using XPS, STM and polarized X-ray absorption spectroscopy reveal that despite their structural similarity they organize very differently on the surface. Furthermore, they exhibit entirely different magnetic anisotropies and hysteresis openings (*cf.* Fig. 1). The relationship between the magnetic, structural and adsorption properties will be discussed.

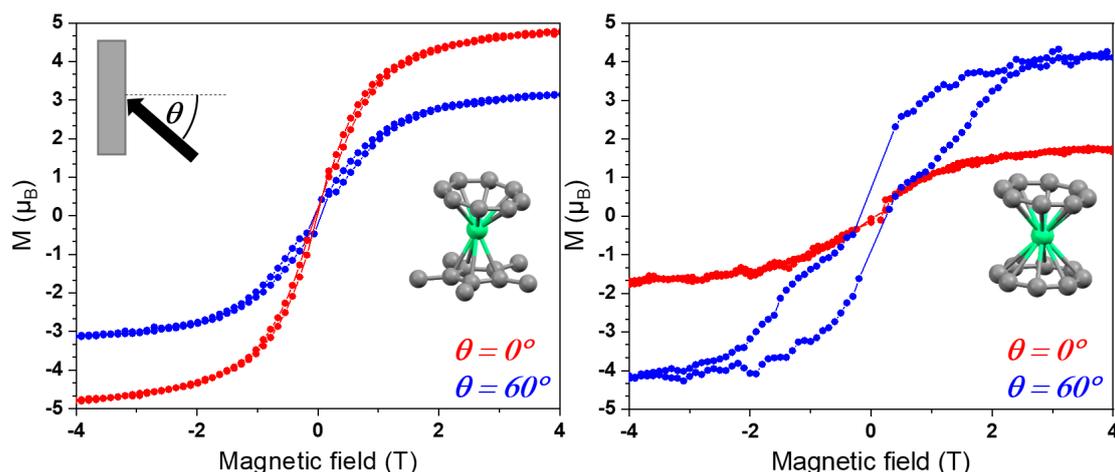


Fig. 1. Magnetic hysteresis loops recorded at  $T = 3$  K on 0.5 monolayers of (left) Cp<sup>\*</sup>ErCOT and (right) Er(COT)<sub>2</sub>. The inset scheme depicts the experimental geometry with the black arrow denoting the incident X-ray beam. In the molecular ball-and-stick images hydrogen and the potassium crown ether counter ion are omitted (color code: grey: carbon; turquoise: erbium). The magnetic anisotropy and the hysteresis opening are entirely different despite the structural similarity of both SMMs.

[1] D. Gatteschi, R. Sessoli, and J. Villain, *Molecular Nanomagnets* (Oxford University Press, 2006)

[2] J. Dreiser, *J. Phys.: Condens. Matter* **27**, 183203 (2015).

[3] C. A. P. Goodwin, F. Ortu, D. Reta, N. F. Chilton, and D. P. Mills, *Nature* **548**, 439 (2017).

[4] F.-S. Guo, B. M. Day, Y.-C. Chen, M.-L. Tong, A. Mansikkamäki, and R. A. Layfield, *Science* **362**, 1400 (2018).

[5] S.-D. Jiang, B.-W. Wang, H.-L. Sun, Z.-M. Wang, and S. Gao, *J. Am. Chem. Soc.* **133**, 4730 (2011).

[6] K. R. Meihaus and J. R. Long, *J. Am. Chem. Soc.* **135**, 17952 (2013).